Methyl 3-butoxypropanoate

4	126-55-0	DTXSID2063395	(

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		75%)	Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.19

Global applicability domain: Inside

Local applicability domain index: 5.37e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

Image not found

2-Isopropyl-6-methyl-4-

pyrimidone Measured: 1.82 Predicted: 2.23 Image not found

Bromacil

Measured: 3.24 Predicted: 2.87

Image not found

Molinate

Measured: 25.7 Predicted: 14.8

Image not found

4-IsobutyImorpholine

Measured: 1.78 Predicted: 2.69

Image not found

Acetamide, N-methyl-N-phenyl-

Measured: 1.51 Predicted: 2.53